



Summerschool on Computational Quantum Chemistry

SCQC-2000 Milano, Italy, July 24-28, 2000

Organized by:

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The goal of the Summerschool (SCQC-2000) is to introduce the participants to the methodologies of modern quantum chemical computation. The course is directed towards young researchers who apply (or who plan on applying) computation to their own research.

The school will mainly focus on practical aspects of computational quantum chemistry, and is built around a kernel of "hands-on" exercises. The exercises are accompanied by a series of lectures which illustrate the methodologies used in the practical assignments. The first three days cover topics of general interest. During the last two days the participants will be free to select practical assignments among the following subjects: Calculations of ESR-NMR Spectra; Molecular Magnetism; Applications of DFT to the calculations of excited states or Ab initio Molecular Dynamics.

Location and Scientific Activity

The first edition of the SCQC was held in Manno (CH), July 27-31, 1998. The second edition will be hosted by CILEA (Consorzio Interuniversitario Lombardo per l'Elaborazione Automatica) in Segrate (MI), Italy.

Current topics in Computational Quantum Chemistry will be covered by lectures:

- Hartree-Fock theory and Electron correlation, H.P. Lüthi, ETHZ, Zurich, CH
- Density Functional Theory A. Goursot, ENSCM, Montpellier, F
- The Potential Energy Surface J. B. Foresman, York College of PA, USA
- Electron Density Analysis and Observables, S. Polezzo, Univ. of Milano-Bicocca, I
- Correlated Methods, P. Fantucci, University of Milano-Bicocca, I
- Solute-Solvent Interactions V. Barone, University of Naples, I
- Molecular Magnetic Properties A. Bencini, University of Florence, I
- NMR and ESR spectroscopy V. Malkin, Slovak Acad. of Science, Bratislava, SL
- Excited States R. Amos, Cambridge University, UK
- Ab initio Molecular Dynamics, A. Sgamellotti, University of Perugia, I

Practical assignment modules will make the students familiar with the use of the best computer programs for solution of chemical problems.

Important Information

On-line information on SCQC-2000 will be found on the web site:

<http://www.cilea.it/Paginecorsi/CSCS/CSCS.htm>

Participants are kindly requested to fill the on-line Registration Form at the same location. The registration fee, which includes accommodation in a student house (23rd-27th July), all lunches and the social banquet.

The number of participants is limited to 40, and an early reservation is needed due to the limited number of rooms available. The deadline for the registration is June 30, 2000.

A few grants, in the form of partial refunding of the registration fee, will be available to young researchers on the basis of their curriculum vitae et studiorum. Application for grants should be made by e-mailing to Prof. P. Fantucci after completing the registration form.